

# Vortex Contribution to Specific Heat of Dirty $d$ -Wave Superconductors: Breakdown of Scaling

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We consider the problem of the vortex contribution to thermal properties of dirty  $d$ -wave superconductors. In the clean limit, the main contribution to the density of states in a  $d$ -wave superconductor arises from extended quasiparticle states which may be treated semiclassically, giving rise to a specific heat contribution  $\delta C(H) \sim H^{1/2}$ . We show that the extended states continue to dominate the dirty limit, but lead to a  $H \log H$  behavior at the lowest fields,  $H_{c1} \lesssim H \ll H_{c2}$ . This crossover may explain recent discrepancies in specific heat measurements at low temperatures and fields in the cuprate superconductors. We discuss the range of validity of recent predictions of scaling with  $H^{1/2}/T$  in real samples.

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*Introduction.* With the growing consensus that the symmetry of the cuprate superconductors is  $d$ -wave [1] has come a renewed interest in the properties of the vortex state in “unconventional” superconductors with order parameter nodes. Many of the basic ideas about how this state differs from the conventional Abrikosov state in classic superconductors were worked out already in the context of rotating  $^3\text{He}$  and heavy fermion superconductors. Recently, however, a number of novel features of the problem peculiar to those systems with Dirac spectrum (line nodes in 3D or point nodes in 2D with order parameter vanishing linearly with angle on the Fermi surface) have been pointed out. Volovik [2] showed that, in contrast to conventional superconductors, extended quasiparticle states with momentum  $\mathbf{k}$  near order parameter nodal directions  $\mathbf{k}_n$  dominate the density of states at zero energy. This leads to a specific heat which varies as  $\delta C(H) \sim H^{1/2}$ , in contrast to classic superconductors, where localized quasiparticle states in vortex cores lead to a scaling of  $\delta C(H) \sim H$  since the number of vortices scales proportionally to the field. Simon and Lee [3] then showed that thermal and transport properties exhibit a scaling with  $H^{1/2}/T$ , again arising simply from the low-energy Dirac form of the electronic spectrum.

The predicted proportionality of the electronic specific heat to  $\sqrt{H}$  was in fact identified in measurements on high quality single crystals by Moler et al., [4] one of the crucial early experiments lending credence to the  $d$ -wave hypothesis. However, the interpretation of the observed  $\sqrt{H}$  dependence has been questioned by Ramirez [5] who points out that there are well-known cases where classic superconductors show a similar “nonanalytic” behavior sufficiently close to the lower critical field  $H_{c1}$ . Furthermore, experimental results of Fisher et al [6] and Revaz et al. [7] cannot be well fit by a  $\sqrt{H}$  form.

The above scaling predictions hold, strictly speaking, for clean  $d$ -wave superconductors and for energy scales small compared to the maximum gap scale  $\Delta_0$ . To make realistic predictions for experiments, deviations from scaling due to disorder and other real-materials effects must be accounted for. In this work, we study the

effects of disorder, primarily in the unitarity scattering limit thought to be relevant to the cuprates, [8,9] and ask how the scaling predictions of refs. [2,3] break down. The treatment is similar in spirit to the crossover phenomena studied in the context of the nonlinear Meissner effect in  $d$ -wave superconductors by Yip and Sauls [10] In the present work we are concerned with fields  $H \gtrsim H_{c1}$ , however, and discuss, in a crude way, the influence of the structure of the vortex state itself on thermodynamic bulk measurements. We analyze existing experiments and point out how they may be reconciled with the  $d$ -wave hypothesis and the ideas of Volovik by properly accounting for the effects of disorder.

*Treatment of extended quasiparticle states.* In an external field, one should in principle solve the Bogoliubov-de Gennes equations or equivalent for the fully self-consistent, spatially dependent mean fields and quasiparticle amplitudes. Imposing a vortex-type boundary condition on the order parameter around an isolated singularity leads to a uniform phase winding with corresponding superfluid velocity  $\mathbf{v}_s = (\hbar/2mr)\hat{\theta}$ , with  $\theta$  the azimuthal angle in real space. The order parameter magnitude  $\Delta_k(\mathbf{R})$  is suppressed near the vortex core over a length scale of order the coherence length  $\xi_0$ , and has a fourfold symmetry in real space. [11] The quasiparticle wavefunctions and quasiparticle density of states have also been claimed [12] to display fourfold symmetry. These excitations are of two types: bound states localized in the vortex cores, and extended states which evolve smoothly into the bulk zero-field quasiparticle states at large distances from the vortex. In a classic superconductor, the low-temperature entropy is dominated by the core bound states, since the extended states are fully gapped and therefore essentially depopulated. The core levels are furthermore separated by a typical spacing  $\Delta_0^2/E_F$ , where  $\Delta_0$  is the gap maximum and  $E_F$  is the Fermi energy. This can be rather large in short-coherence length superconductors like the cuprates, such that only one or a few states may actually be bound. Even if treated as a quasicontinuum, in a  $d$ -wave superconductor the bound states may be shown to contribute less to

the entropy than the extended states with momenta near the bulk gap nodal directions, [2] by an amount which diverges logarithmically with the vortex size or intervortex separation. Since nonmagnetic disorder is pairbreaking in a d-wave superconductor, the contribution of low-energy extended states to the entropy will be still greater in the dirty systems we consider.

For the above reasons, it appears in the *d*-wave case to be a good approximation to ignore the core excitations in the calculation of bulk properties. The extended excitations are treated here by a method originally proposed by Maki and Tsuneto [13] for classic superconductors and applied to the d-wave nonlinear Meissner effect by Yip and Sauls. [10] The semiclassical approximation treats the quasiparticle states as plane waves of energy Doppler shifted by  $\omega \rightarrow \omega - \mathbf{v}_s \cdot \mathbf{k}$ . The single-particle matrix Green's function for the pure system is therefore

$$g^{(0)}(\mathbf{k}, \omega; \mathbf{v}_s) = \frac{(\omega - \mathbf{v}_s \cdot \mathbf{k})\tau_0 + \Delta_{\mathbf{k}}\tau_1 + \xi_{\mathbf{k}}\tau_3}{(\omega - \mathbf{v}_s \cdot \mathbf{k})^2 - \Delta_{\mathbf{k}}^2 - \xi_{\mathbf{k}}^2}, \quad (1)$$

where the  $\tau_i$  are Pauli matrices in particle-hole space. In (1),  $\xi_{\mathbf{k}}$  is the usual single-particle band measured relative to the Fermi level, and  $\Delta_{\mathbf{k}} = \Delta_0 \cos 2\phi$  is the bulk  $d_{x^2-y^2}$  order parameter over a cylindrical Fermi surface, taken independent of position in real space. Thus, we neglect both the order parameter suppression and the spatial variation of the quasiparticle amplitudes near the vortex core over the coherence length  $\xi_0 = \hbar v_F / \pi \Delta_0$ . This is justified provided we confine our interest to fields  $H$  such that  $H_{c1} \lesssim H \ll H_{c2}$ : the coherence length  $\xi_0$  will then be much smaller than the other relevant length scales, specifically  $R$ , the intervortex distance and  $\lambda$ , the penetration depth, in a strongly type-II system.

Disorder is introduced in the self-consistent t-matrix approximation [14,15] through the averaged self-energy  $\Sigma_0(\omega) = \Gamma G_0 \tau_0 / (c^2 - G_0^2)$ , where  $\Gamma = n_i / \pi N_0$  is an impurity scattering rate proportional to the concentration  $n_i$  of point potential scatterers,  $c = \cot \delta_0$  is the cotangent of the s-wave scattering phase shift  $\delta_0$ , and  $N_0$  is the density of states at the Fermi level. We focus here on the strong scattering limit  $\delta_0 \simeq \pi/2$ , but results are easily obtained for general phase shifts. The averaged integrated Green's function is  $G_0(\omega) = (\pi N_0)^{-1} \Sigma_{\mathbf{k}} \frac{1}{2} \text{Tr} \tau_0 g(\mathbf{k}, \omega)$ , which for a simple  $d_{x^2-y^2}$  state leads to  $G_0(\omega) = -i(2/\pi) \mathbf{K}(\Delta_0/\tilde{\omega})$ . This form of the self-energy leads via the Dyson equation to an averaged propagator  $g(\mathbf{k}, \omega)$  identical in form to (1) but with  $\omega$  replaced by  $\tilde{\omega} = \omega - \Sigma_0(\omega)$ . Note the Green's function must be determined self-consistently, and depends on the single energy variable  $\tilde{\omega} - \mathbf{v}_s \cdot \mathbf{k}$ . It is furthermore important to observe that the most general form of the propagator would include renormalizations of both the single-particle energy  $\xi_{\mathbf{k}}$  and the order parameter  $\Delta_{\mathbf{k}}$  as well. Corrections due to the former vanish identically for one-particle properties like the density of states if the system is particle-hole symmetric. [16] Corrections due to the latter, which vanish for a  $d_{x^2-y^2}$  order parameter in the  $H = 0$  case, are nonzero in general in finite field, due

to the dependence of the shift  $\mathbf{v}_s \cdot \mathbf{k}$  on the angle  $\phi$  over the Fermi surface. However, for low energies such that only quasiparticles in the neighborhood of the nodes are relevant, this renormalization may be shown to be small, and we have neglected it here.

*Density of states at zero energy in nonzero field.* We first present results for the magnetic field dependence of the density of states at zero energy,  $N(0; H)$ . This is an experimentally accessible quantity, as it scales with the linear-T term in the low-temperature specific heat in the superconducting state,  $\gamma_{el} = \pi^2 N(0)/3$ . The origin of this term has been controversial, and may result in part from nonelectronic two-level systems away from the planes. The zero-field residual density of states used in this work arises solely through disorder in the electronic system, and must be assumed to represent a lower bound to the true residual density of states. To find  $N(0; H)$ , we average the propagator over a vortex unit cell,  $N(0; H)/N_0 \equiv \langle -\text{Im} G_0(\omega; \mathbf{v}_s) \rangle_H$ , where for any  $f(\mathbf{v}_s)$  we define  $\langle f(\mathbf{v}_s) \rangle_H \equiv A^{-1}(H) \int_{\text{cell}} d^2r f(\mathbf{v}_s)$ . For simplicity, we take the cell to be circular, of area  $A \simeq \pi R^2$ . Here  $R = \xi_0(\pi/2)^{1/2} a^{-1} (H_{c2}/H)^{1/2}$  is the intervortex spacing, and  $a$  is a constant of order unity dependent only on the vortex lattice geometry. Note that increasing the magnetic field does not affect  $\mathbf{v}_s$ , but merely decreases  $R$ . Effects of the actual spatial dependence of  $\mathbf{v}_s$  in the lattice phase can be easily incorporated in the theory.

In the clean limit and for  $H_{c1} \lesssim H \ll H_{c2}$ , we obtain  $N(0; H)/N_0 \simeq \sqrt{8/\pi a} (H/H_{c2})^{1/2}$ . This is essentially the result obtained by Volovik, [2] who linearized the gap and the electronic spectrum around the nodes, and may be derived easily by recalling that for the  $d_{x^2-y^2}$  state  $N(\omega)/N_0 \simeq \omega/\Delta_0$  for  $\omega \ll \Delta_0$ , replacing  $\omega$  by  $\mathbf{v}_s \cdot \mathbf{k}$ , and performing the spatial integral over the cell. This approximation must therefore fail at low energies, where the density of states in the disordered  $H = 0$  system has the form  $N(\omega) \sim N(0) + b\omega^2$ , with  $N(0)$  related to the zero-energy quasiparticle scattering rate  $2\gamma_0$  by  $N(0) = (2\gamma_0/\pi\Delta_0) \log(4\Delta_0/\gamma_0)$ . In the unitarity limit,  $\gamma_0$  is well approximated by  $\gamma_0 \simeq 0.61\sqrt{\Gamma\Delta_0}$  for small concentrations.

As in the zero-field case above, the residual density of states depends on the quasiparticle lifetime, which becomes, however, a local quantity in the presence of the superflow field  $\mathbf{v}_s(\mathbf{r})$ . At low energies, substitution of the form  $\tilde{\omega}(\mathbf{r}) = \omega + i\gamma(\mathbf{r})$  into  $\Sigma_0(\omega)$  yields for  $v_s k_F, \gamma \ll \Delta_0$  but arbitrary  $v_s k_F/\gamma$ ,

$$\frac{\gamma}{\Delta_0} = \frac{\pi}{2} \frac{\Gamma}{\Delta_0} \left[ \ln \left( \frac{4\Delta_0}{\sqrt{\gamma^2 + (\mathbf{v}_s \cdot \mathbf{k}_n)^2}} \right) + \frac{\mathbf{v}_s \cdot \mathbf{k}_n}{\gamma} \tan^{-1} \left( \frac{\mathbf{v}_s \cdot \mathbf{k}_n}{\gamma} \right) \right]^{-1}, \quad (2)$$

where  $\mathbf{k}_n$  is the nodal direction. In the “dirty limit”,  $(H/H_{c2})^{1/2} \Delta_0 \ll \gamma_0 \ll \Delta_0$ , the spatial integrations in  $\langle -\text{Im} G_0 \rangle_H$  can be performed, yielding

$$\frac{\delta N(0, H)}{N_0} \simeq \frac{\Delta_0}{8\gamma_0} a^2 \left( \frac{H}{H_{c2}} \right) \log \left[ \frac{\pi}{2a^2} \left( \frac{H_{c2}}{H} \right) \right] \quad (3)$$

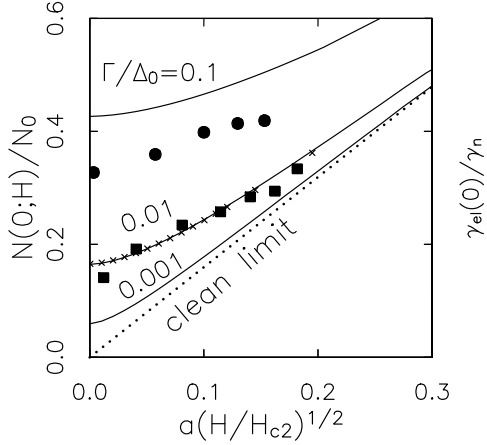


FIG. 1. Normalized density of states  $N(0;H)/N_0$  for  $\Gamma/\Delta_0 = 0.1, 0.01$ , and  $0.001$  in unitarity limit  $c = 0$ . Nodal approximation (solid lines), exact result (crosses), clean, low energy approximation (dotted line). Data from Fisher et al. [6] (circles); Moler et al. [4] (untwinned sample, squares), assuming  $H_{c2}/a^2 = 300\text{T}$ ,  $\gamma_n = 15 \text{ mJ-mol-K}^2$ .

To illustrate the deviations from the clean limit, low-energy result, we plot in Figure 1 a full numerical evaluation of the density of states  $N(0;H)$ . For the cleanest case plotted, the predicted scaling is attained over a substantial range. Deviations from the  $\sqrt{H}$  behavior occur below a lower crossover field scale  $H^* \equiv (\gamma_0/a\Delta_0)^2 H_{c2}$ , corresponding to the smearing of the linear density of states due to scattering by impurities. We note that excellent approximate results may be obtained, with a substantial increase in speed of numerical evaluation, by replacing  $\mathbf{v}_s \cdot \mathbf{k}$  in  $g(\mathbf{k}, \omega; \mathbf{v}_s)$  by its value near the nodes,  $\mathbf{v}_s \cdot \mathbf{k}_n$ , so that  $G_0(\omega; \mathbf{v}_s) \simeq (1/\pi) \sum_{\alpha=\pm} \mathbf{K}(\Delta_0/(\tilde{\omega} - \alpha \mathbf{v}_s \cdot \mathbf{k}_n))$ . We use this approximate form, whose validity is shown in Figure 1, in all further calculations.

In Figure 1 we have also shown experimental data of Moler et al. [4] and Fisher et al. [6]. We have plotted published data for the linear electronic specific heat coefficient  $\gamma_{el}$  without attempting to subtract residual “extrinsic” contributions possibly due to 2-level systems, etc. We observe that the data for the untwinned YBCO crystal of Moler et al., which are claimed to follow the clean-limit prediction of Volovik, [2] are actually consistent with a slightly dirty  $d$ -wave superconductor as well if the entire residual contribution to  $N(0;H)$  is attributed to impurities (analysis of NMR and penetration depth data on similar samples makes this interpretation unlikely, however. [4]). No good fit to the clean limit prediction was obtained for the sample studied by Fisher et al. From the Figure it is clear that this discrepancy might be explained by simply assuming the Fisher et al. sample contains roughly an order of magnitude more defects than the Moler et al. sample. Clearly systematic

disorder studies would be very useful in resolving these questions.

*Density of states at finite frequency.* Kopnin and Volovik [17] have observed that the field-dependent part of the density of states,  $\delta N(\omega; H)$  will diverge at low frequencies as  $1/\omega$  down to a lower cutoff of order the average quasiparticle energy shift  $E_H \equiv a(H/H_{c2})^{1/2} \Delta_0$ . In the current formalism, this result is recovered by noting that the field-dependent part of the local density of states is given by  $\langle -\text{Im}[G_0(\omega; \mathbf{v}_s) - G_0(\omega)] \rangle_H$ , which for  $\gamma_0 < E_H, \omega \ll \Delta_0$  yields

$$\frac{\delta N(\omega; H)}{N_0} \simeq \left\langle \left| \frac{\mathbf{v}_s \cdot \mathbf{k}_n - \omega}{\Delta_0} \right| - \left| \frac{\omega}{\Delta_0} \right| \right\rangle_H \simeq \frac{E_H}{\sqrt{2\pi}\Delta_0^2} F(x) \quad (4)$$

$$F(x) \equiv \frac{1}{x} \begin{cases} \pi/2 & x > 1 \\ 3x\sqrt{1-x^2} + (1+2x^2)\sin^{-1}x - \pi x^2 & x < 1 \end{cases}$$

where  $x = \sqrt{2/\pi}(\omega/E_H)$ . The desired result is then

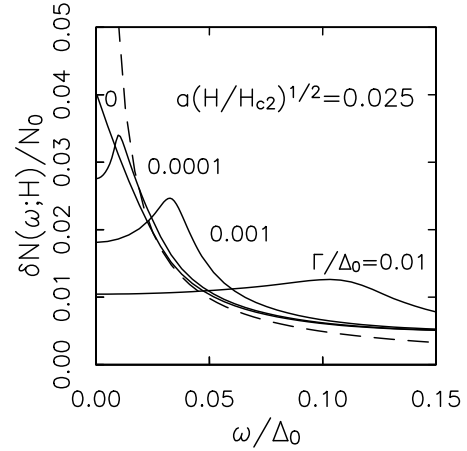


FIG. 2. Density of states at  $a(H/H_{c2})^{1/2} = 0.025$  vs. freq.  $\omega/\Delta_0$  for  $\Gamma/T_c = 0, 0.0001, 0.001, 0.01$  (solid lines). Intermediate-frequency asymptotic result  $\delta N \simeq a^2 \pi \Delta_0 H / (4\omega H_{c2})$  (dashed line).

obtained in the limit of large frequencies,  $\delta N(\omega; H)/N_0 \simeq a^2 \pi \Delta_0 H / (4\omega H_{c2})$ . At energies smaller than the average quasiparticle energy shift  $E_H$ , this divergence is cut off as  $\delta N(\omega; H) \simeq N(0; H)(1 - \pi x/4)$ . Both these limits are clearly visible in the clean case shown in Figure 2. The  $1/\omega$  divergence may also be cut off in a different fashion if the impurity scale  $\gamma_0$  exceeds the magnetic energy,  $E_H < \omega < \gamma_0$ , as also shown (the maximum in each curve corresponds roughly to the scale  $\gamma_0$ ). In dirty samples, such that  $\gamma_0$  becomes an appreciable fraction of the gap scale, the  $1/\omega$  behavior will be unobservable.

*$H^{1/2}/T$  scaling of specific heat.* The specific heat is now easy to calculate by differentiating the entropy of a free Fermi gas of quasiparticles with disorder- and field-averaged density of states  $N(\omega; H)$ ; one finds at low temperatures:

$$C \simeq 2 \int_0^\infty d\omega \left(\frac{\omega}{T}\right)^2 \left(\frac{-\partial f}{\partial \omega}\right) N(\omega; H) \quad (5)$$

$$\simeq \begin{cases} N(0; H) \frac{\pi^2}{3} T & T \ll \max[\gamma_0, E_H] \ll \Delta_0 \\ N_0 \left(\frac{9\zeta(3)}{\Delta_0}\right) T^2 & \gamma_0, E_H \ll T \ll \Delta_0 \end{cases}$$

A  $T^2$  term characteristic of the pure  $d$ -wave system in zero field is present whenever both the impurity and magnetic field scales are smaller than the temperature. If one

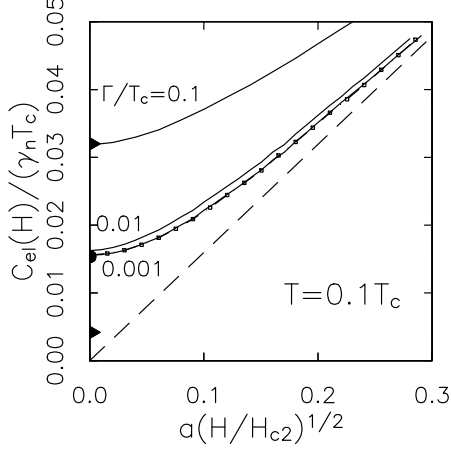


FIG. 3. Electronic specific heat  $C_{el}(H)/(\gamma_n T_c)$  at  $T = 0.1 T_c$  normalized to normal state value,  $\gamma_n T_c$  vs. square root of field,  $a(H/H_{c2})^{1/2}$  for  $\Gamma/T_c = 0.1, 0.01$  and  $0.001$  (solid lines). Clean limit (small filled circles). Asymptotic low- $T$  clean limit (dashed line). Zero-field linear term  $N(0;0)T$  (filled triangles) for values of  $\Gamma$  shown.

plots the specific heat at fixed temperature, as in Fig. 3, this results at low fields in deviations from  $\sqrt{H}$  behavior due both to impurity induced residual density of states and, in cleaner samples, the  $T^2$  term. The latter effect is the origin of the saturation of the progressively cleaner curves in the figure to a non- $\sqrt{H}$  behavior.

Finally, we examine the scaling behavior predicted for the specific heat. [3,18] In the clean, low-energy limit,

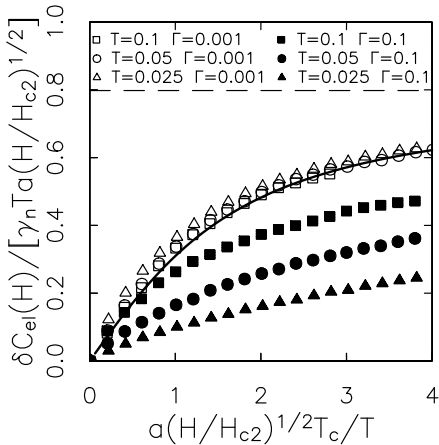


FIG. 4. Normalized vortex contribution to specific heat,  $\delta C_{el}(H)/[\gamma_n T a(H/H_{c2})^{1/2}]$  vs.  $Y \equiv a(H/H_{c2})^{1/2} T_c/T$  for fixed temperatures  $T$  and scattering rates  $\Gamma$  as shown; unit of energy  $T_{c0}$ . Asymptotic large- $Y$  limit  $\sqrt{2/\pi}$  (dashed line).

this result may be derived by substituting Eq. (4) into (5). One finds  $\delta C(H)/[\gamma_n T a(H/H_{c2})^{1/2}] = F_C[Y]$ , where  $Y = a(H/H_{c2})^{1/2} T_c/T$  and  $F_C$  is a scaling function which varies as  $F_C \simeq 3 \log 2 \Delta_0 Y / (4\pi T_c)$  for  $Y \ll 1$  and as  $F_C \simeq \sqrt{2/\pi}$  for  $Y \gg 1$ . The full numerically determined, low-energy clean limit scaling function is plotted in Figure 4, along with full numerical evaluations of (5), which includes corrections beyond the low-energy approximation, as well as impurity effects. Scaling is expected for a given data set provided  $H, T$  are such that  $E_H$  and  $T$  are both larger than the impurity scale  $\gamma$ . For example, in the clean case chosen (open symbols), scaling is obtained over the full range of  $Y$ , whereas for the dirty system (filled symbols) scaling has broken down completely. Junod [19] has recently reported data which crudely follow scaling predictions, but scatter in the data is too great to ascertain if the deviations follow the pattern predicted here.

**Conclusions.** We have placed the elegant scaling arguments of Volovik [2,18] and Simon and Lee [3] regarding the specific heat of a  $d$ -wave superconductor in magnetic field on a concrete foundation, introducing a simple formalism capable of including both the effects of disorder and of energies comparable to the gap scale. We have shown that the density of states of a dirty  $d$ -wave system varies as  $H \log H$  rather than the  $\sqrt{H}$  expected for the clean system. As a result, the predicted scaling of the vortex specific heat  $\delta C(H)$  with  $\sqrt{H}/T$  breaks down in a well-defined fashion. As sample variability in the cuprates is notorious, it will be important to understand these deviations. We are in the process of studying similar effects in transport properties in a magnetic field.

*Note added:* After submission of this paper we learned that Y. Barash et al. [20] had also obtained Eq. (3). We are grateful to G.E. Volovik for pointing out this reference.

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